Package ‘SingleCellMultiModal’

April 4, 2024

Type Package

Title Integrating Multi-modal Single Cell Experiment datasets

Version 1.14.0

Description SingleCellMultiModal is an ExperimentHub package that serves multiple datasets obtained from GEO and other sources and represents them as MultiAssayExperiment objects. We provide several multi-modal datasets including scNMT, 10X Multiome, seqFISH, CITeseq, SCoPE2, and others. The scope of the package is to provide data for benchmarking and analysis.

License Artistic-2.0

BugReports https://github.com/waldronlab/SingleCellMultiModal/issues

Depends R (>= 4.2.0), MultiAssayExperiment

Imports AnnotationHub, BiocBaseUtils, BiocFileCache, ExperimentHub, graphics, HDF5Array, S4Vectors, SingleCellExperiment, SpatialExperiment, SummarizedExperiment, Matrix, methods, utils

Suggests BiocStyle, ggplot2, knitr, RaggedExperiment, rmarkdown, scater, scran, UpSetR, uwot

VignetteBuilder knitr

biocViews ExperimentData, SingleCellData, ReproducibleResearch, ExperimentHub, GEO

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**R topics documented:**

- `SingleCellMultiModal-package` ................................................................. 2
- `.CITEseqMaeToSce` .................................................................................. 3
- `addCTLabels` ............................................................................................ 4
- `CITEseq` ..................................................................................................... 5
- `getCellGroups` ........................................................................................... 7
- `GTseq` ......................................................................................................... 8
- `ontomap` ....................................................................................................... 9
- `scnmCache` ................................................................................................ 10
- `scMultiome` ............................................................................................... 11
- `scNMT` ......................................................................................................... 12
- `SCoPE2` ...................................................................................................... 14
- `seqFISH` ...................................................................................................... 16
- `SingleCellMultiModal` ............................................................................... 17

**Index**

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`SingleCellMultiModal-package`

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**Description**

The `SingleCellMultiModal` package provides a convenient and user-friendly representation of multimodal data from project such as ‘scNMT’ for mouse gastrulation.

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\textbf{Description}

converts a ‘MultiAssayExperiment’ object with CITEseq data into a ‘SingleCellExperiment’ object to be used with already known methods and packages in literature.

Note that for creating a ‘SingleCellExperiment’ object the following function subsets all the assays present in the ‘MultiAssayExperiment’ with only the common cells across all the modalities. This could result in a not complete object.

\textbf{Usage}

\texttt{.CITEseqMaeToSce(mae)}

\textbf{Arguments}

\texttt{mae} \\
\hspace{1em} a MultiAssayExperiment object with scRNA and/or scADT and/or scHTO named experiments.

\textbf{Value}

a SingleCellExperiment object as widely with scRNA data as counts and scADT, scHTO data as altExps. If only one modality is present, it has returned as main assay of the SCE.
addCTLabels

Description

addCTLabels

Usage

addCTLabels(
  cd,
  out,
  outname,
  ct,
  mkrcol = "markers",
  ctcol = "celltype",
  overwrite = FALSE,
  verbose = TRUE
)

Arguments

- cd: the colData DataFrame
- out: list data structure returned by getCellGroups
- outname: character indicating the name of the out data structure
- ct: character indicating the celltype to assign in the ctcol
- mkrcol: character indicating the cd column to store the markers indicated by outname (default is markers)
- ctcol: character indicating the column in cd to store the cell type indicated by ct (default is celltype)
- overwrite: logical indicating if the cell types have to be overwritten without checking if detected barcodes were already assigned to other celltypes
- verbose: logical for having informative messages during the execution

Value

an updated version of the cd DataFrame
Description

function assembles data on-the-fly from ‘ExperimentHub’ to provide a MultiAssayExperiment container. Actually the ‘dataType’ argument provides access to the available datasets associated to the package.

Usage

CITEseq(
  DataType = c("cord_blood", "peripheral_blood"),
  modes = "*",
  version = "1.0.0",
  dry.run = TRUE,
  filtered = FALSE,
  verbose = TRUE,
  DataClass = c("MultiAssayExperiment", "SingleCellExperiment"),
  ...
)

Arguments

DataType character(1) indicating the identifier of the dataset to retrieve. (default "cord_blood")

modes character() The assay types or modes of data to obtain these include scADT and scRNA-seq data by default.

version character(1) Either version ‘1.0.0’ depending on data version required.

dry.run logical(1) Whether to return the dataset names before actual download (default TRUE)

filtered logical(1) indicating if the returned dataset needs to have filtered cells. See Details for additional information about the filtering process.

verbose logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)

DataClass either MultiAssayExperiment or SingleCellExperiment data classes can be returned (default MultiAssayExperiment)

Details

CITEseq data are a combination of single cell transcriptomics and about a hundred of cell surface proteins.

Available datasets are:

• cord_blood: a dataset of single cells of cord blood as provided in Stoeckius et al. (2017).
- scRNA_Counts - Stoeckius scRNA-seq gene count matrix
- scADT - Stoeckius antibody-derived tags (ADT) data

• peripheral_blood: a dataset of single cells of peripheral blood as provided in Mimitou et al. (2019). We provide two different conditions controls (CTRL) and Cutaneous T-cell Lymphoma (CTCL). Just build appropriate modes regex for subselecting the dataset modes.
  - scRNA - Mimitou scRNA-seq gene count matrix
  - scADT - Mimitou antibody-derived tags (ADT) data
  - scHTO - Mimitou Hashtag Oligo (HTO) data
  - TCRab - Mimitou T-cell Receptors (TCR) alpha and beta available through the object metadata.
  - TCRgd - Mimitou T-cell Receptors (TCR) gamma and delta available through the object metadata.

If ‘filtered’ parameter is ‘FALSE’ (default), the ‘colData’ of the returned object contains multiple columns of ‘logicals’ indicating the cells to be discarded. In case ‘filtered’ is ‘TRUE’, the ‘discard’ column is used to filter the cells. Column ‘adt.discard’ indicates the cells to be discarded computed on the ADT assay. Column ‘mito.discard’ indicates the cells to be discarded computed on the RNA assay and mitochondrial genes. Column ‘discard’ combines the previous columns with an ‘OR’ operator. Note that for the ‘peripheral_blood’ dataset these three columns are computed and returned separately for the ‘CTCL’ and ‘CTRL’ conditions. In this case the additional ‘discard’ column combines the ‘discard.CTCL’ and ‘discard.CTRL’ columns with an ‘OR’ operator. Cell filtering has been computed for ‘cord_blood’ and ‘peripheral_blood’ datasets following section 12.3 of the Advanced Single-Cell Analysis with Bioconductor book. Executed code can be retrieved in the CITEseq_filtering.R script of this package.

Value

A single cell multi-modal MultiAssayExperiment or informative ‘data.frame’ when ‘dry.run’ is ‘TRUE’. When ‘DataClass’ is ‘SingleCellExperiment’ an object of this class is returned with an RNA assay as main experiment and other assay(s) as ‘AltExp(s)’.

Author(s)

Dario Righelli

References

Stoeckius et al. (2017), Mimitou et al. (2019)

Examples

mae <- CITEseq(DataType="cord_blood", dry.run=FALSE)
experiments(mae)
getCellGroups

Description

Shows the cells/barcodes in two different plots (scatter and density) dividing the space in four quadrant indicated by the two thresholds given as input parameters. The x/y-axis represent respectively the two ADTs given as input. It returns a list of one element for each quadrant, each with barcodes and percentage (see Value section for details).

Usage

getCellGroups(mat, adt1 = "CD19", adt2 = "CD3", th1 = 0.2, th2 = 0)

Arguments

mat matrix of counts or clr transformed counts for ADT data in CITEseq
adt1 character indicating the name of the marker to plot on the x-axis (default is CD19).
adt2 character indicating the name of the marker to plot on the y-axis (default is CD3).
 th1 numeric indicating the threshold for the marker on the x-axis (default is 0.2).
 th2 numeric indicating the threshold for the marker on the y-axis (default is 0).

Details

helps to do manual gating for cell type indentification with CITEseq or similar data, providing cell markers. Once identified two interesting markers for a cell type, the user has to play with the thresholds to identify the cell populations specified by an uptake (+) o downtake (-) of the couple of markers (ADTs) previously selected.

Value

a list of four different element, each one indicating the quarter where the thresholds divide the plotting space, in euclidean order I, II, III, IV quadrant, indicating respectively +/-, +/-, -/-, -/- combinations for the couples of selected ADTs. Each element of the list contains two objects, one with the list of detected barcodes and one indicating the percentage of barcodes falling into that quadrant.
GTseq

Parallel sequencing data of single-cell genomes and transcriptomes

Description

GTseq assembles data on-the-fly from ExperimentHub to provide a MultiAssayExperiment container. The DataType argument provides access to the mouse_embryo_8_cell dataset as obtained from Macaulay et al. (2015). Protocol information for this dataset is available from Macaulay et al. (2016). See references.

Usage

GTseq(
  DataType = "mouse_embryo_8_cell",
  modes = "*",
  version = "1.0.0",
  dry.run = TRUE,
  verbose = TRUE,
  ...
)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DataType</td>
<td>character(1) Indicates study that produces this type of data (default: 'mouse_embryo_8_cell')</td>
</tr>
<tr>
<td>modes</td>
<td>character() A wildcard / glob pattern of modes, such as &quot;<em>omic&quot;. A wildcard of &quot;</em>&quot; will return all modes including copy numbers (&quot;genomic&quot;) and RNA-seq read counts (&quot;transcriptomic&quot;), which is the default.</td>
</tr>
<tr>
<td>version</td>
<td>character(1). Currently, only version '1.0.0'.</td>
</tr>
<tr>
<td>dry.run</td>
<td>logical(1) Whether to return the dataset names before actual download (default TRUE)</td>
</tr>
<tr>
<td>verbose</td>
<td>logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)</td>
</tr>
<tr>
<td>...</td>
<td>Additional arguments passed on to the ExperimentHub-class constructor</td>
</tr>
</tbody>
</table>

Details

G&T-seq is a combination of Picoplex amplified gDNA sequencing (genome) and SMARTSeq2 amplified cDNA sequencing (transcriptome) of the same cell. For more information, see Macaulay et al. (2015).

- mouse_embryo_8_cell: this dataset was filtered for bad cells as specified in Macaulay et al. (2015).
  - genomic - integer copy numbers as detected from scDNA-seq
  - transcriptomic - raw read counts as quantified from scRNA-seq
ontomap

Value
A single cell multi-modal MultiAssayExperiment or informative data.frame when dry.run is TRUE.

metadata
The MultiAssayExperiment metadata includes the original function call that saves the function call and the data version requested.

Source
https://www.ebi.ac.uk/ena/browser/view/PRJEB9051

References

See Also
SingleCellMultiModal-package

Examples
GTseq()

---

ontomap Obtain a map of cell types for each dataset

Description
The ‘ontomap’ function provides a mapping of all the cell names across the all the data sets or for a specified data set.

Usage
ontomap(dataset = c("scNMT", "scMultiome", "SCOPE2", "CITEseq", "seqFISH"))

Arguments
dataset 'character()' One of the existing functions within the package. If missing, a map of all cell types in each function will be provided.
Details

Note that 'CITEseq' does not have any cell annotations; therefore, no entries are present in the 'ontomap'.

Value

A 'data.frame' of metadata with cell types and ontologies

Examples

```r
ontomap(dataset = 'scNMT')
```

---

**scmmCache**  
*Manage cache / download directories for study data*

Description

Managing data downloads is important to save disk space and re-downloading data files. This can be done effortlessly via the integrated BiocFileCache system.

Usage

```r
scmmCache(...)  
setCache(  
directory = tools::R_user_dir("SingleCellMultiModal", "cache"),  
verbose = TRUE,  
ask = interactive()  
)
```

Arguments

- `...`: For `scmmCache`, arguments passed to `setCache`
- `directory`: character(1) The file location where the cache is located. Once set, future downloads will go to this folder. See `setCache` section for details.
- `verbose`: Whether to print descriptive messages
- `ask`: logical(1) (default TRUE when `interactive()`) Confirm the file location of the cache directory
- `accession`: character(1) A single string indicating the accession number of the study

Value

The directory / option of the cache location
**scMultiome**

**scmmCache**

Get the directory location of the cache. It will prompt the user to create a cache if not already created. A specific directory can be used via `setCache`.

**setCache**

Specify the directory location of the data cache. By default, it will go into the user’s home and package name directory as given by `R_user_dir` (default: varies by system e.g., for Linux: `$HOME/.cache/R/SingleCellMultiModal`).

**removeCache**

Some files may become corrupt when downloading, this function allows the user to delete the tarball associated with a study number in the cache.

**Examples**

```r
getOption("scmmCache")
scmCache()
```

---

**scMultiome**  
*Single-cell Multiome ATAC + Gene Expression*

**Description**

10x Genomics Multiome technology enables simultaneous profiling of the transcriptome (using 3’ gene expression) and epigenome (using ATAC-seq) from single cells to deepen our understanding of how genes are expressed and regulated across different cell types. Data prepared by Ricard Argelaguet.

**Usage**

```r
scMultiome(
  DataType = "pbmc_10x",
  modes = "*",
  version = "1.0.0",
  format = c("MTX", "HDF5"),
  dry.run = TRUE,
  verbose = TRUE,
  ...
)
```
Arguments

**DataType**
character(1) Indicates study that produces this type of data (default: 'mouse_gastrulation')

**modes**
character() A wildcard / glob pattern of modes, such as "acc*". A wildcard of "*" will return all modes including Chromatin Accessibility ("acc"), Methylation ("met"), RNA-seq ("rna") which is the default.

**version**
character(1) Either version '1.0.0' or '2.0.0' depending on data version required (default '1.0.0'). See version section.

**format**
Either MTX or HDF5 data format (default MTX)

**dry.run**
logical(1) Whether to return the dataset names before actual download (default TRUE)

**verbose**
logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)

... Additional arguments passed on to the `ExperimentHub-class` constructor

Details

Users are able to choose from either an MTX or HDF5 file format as the internal data representation. The MTX (Matrix Market) format allows users to load a sparse `dgCMatrix` representation. Choosing HDF5 gives users a sparse `HDF5Array` class object.

`pbmc_10x`:

10K Peripheral Blood Mononuclear Cells provided by [10x Genomics website](https://www.10xgenomics.com) Cell quality control filters are available in the object `colData` together with the `celltype` annotation labels.

Value

A 10X PBMC MultiAssayExperiment object

Examples

```r
scMultiome(DataType = "pbmc_10x", modes = "*", dry.run = TRUE)
```

---

**scNMT**

*Single-cell Nucleosome, Methylation and Transcription sequencing*

Description

scNMT assembles data on-the-fly from ExperimentHub to provide a MultiAssayExperiment container. The `DataType` argument provides access to the mouse_gastrulation dataset as obtained from Argelaguet et al. (2019; DOI: 10.1038/s41586-019-1825-8). Pre-processing code can be seen at [https://github.com/rargelaguet/scnmt_gastrulation](https://github.com/rargelaguet/scnmt_gastrulation). Protocol information for this dataset is available at Clark et al. (2018). See the vignette for the full citation.
Usage

```r
scNMT(
  DataType = "mouse_gastrulation",
  modes = "*",
  version = "1.0.0",
  dry.run = TRUE,
  verbose = TRUE,
  ...
)
```

Arguments

- **DataType** character(1) Indicates study that produces this type of data (default: 'mouse_gastrulation')
- **modes** character() A wildcard / glob pattern of modes, such as "acc*". A wildcard of "*" will return all modes including Chromatin Accessibilty ("acc"), Methylation ("met"), RNA-seq ("rna") which is the default.
- **version** character(1) Either version '1.0.0' or '2.0.0' depending on data version required (default '1.0.0'). See version section.
- **dry.run** logical(1) Whether to return the dataset names before actual download (default TRUE)
- **verbose** logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)
- **...** Additional arguments passed on to the ExperimentHub-class constructor

Details

scNMT is a combination of RNA-seq (transcriptome) and an adaptation of Nucleosome Occupancy and Methylation sequencing (NOMe-seq, the methylome and chromatin accessibility) technologies. For more information, see Reik et al. (2018) DOI: 10.1038/s41467-018-03149-4

- **mouse_gastrulation**: this dataset provides cell quality control filters in the object colData starting from version 2.0.0. Additionally, cell types annotations are provided through the lineage colData column.
  - rna - RNA-seq
  - acc_ - chromatin accessibility met_ - DNA methylation
    * cgi - CpG islands
    * CTCF - footprints of CTCF binding
    * DHS - DNase Hypersensitive Sites
    * genebody - gene bodies
    * p300 - p300 binding sites
    * promoter - gene promoters

Special thanks to Al J Abadi for preparing the published data in time for the 2020 BIRS Workshop, see the link here: urlhttps://github.com/BIRSBiointegration/Hackathon/tree/master/scNMT-seq
Value

A single cell multi-modal MultiAssayExperiment or informative data.frame when dry.run is TRUE.

versions

Version '1.0.0' of the scNMT mouse_gastrulation dataset includes all of the above mentioned assay technologies with filtering of cells based on quality control metrics. Version '2.0.0' contains all of the cells without the QC filter and does not contain CTCF binding footprints or p300 binding sites.

metadata

The MultiAssayExperiment metadata includes the original function call that saves the function call and the data version requested.

Source

http://ftp.ebi.ac.uk/pub/databases/scnmt_gastrulation/

References

Argelaguet et al. (2019)

See Also

SingleCellMultiModal-package

Examples

```r
scNMT(DataType = "mouse_gastrulation", modes = "]", version = "1.0.0", dry.run = TRUE)
```

---

**SCoPE2**

*Single-cell RNA sequencing and proteomics*

**Description**

SCoPE2 assembles data on-the-fly from ExperimentHub to provide a MultiAssayExperiment container. The DataType argument provides access to the SCoPE2 dataset as provided by Specht et al. (2020; DOI: http://dx.doi.org/10.1101/665307). The article provides more information about the data acquisition and pre-processing.
Usage

SCoPE2(
  DataType = "macrophage_differentiation",
  modes = "*",
  version = "1.0.0",
  dry.run = TRUE,
  verbose = TRUE,
  ...
)

Arguments

- **DataType**: character(1) Indicates study that produces this type of data (default: 'macrophage_differentiation')
- **modes**: character() A wildcard / glob pattern of modes, such as "rna". A wildcard of "*" will return all modes, that are transcriptome ("rna") or proteome ("protein") which is the default.
- **version**: character(1), currently only version '1.0.0' is available
- **dry.run**: logical(1) Whether to return the dataset names before actual download (default TRUE)
- **verbose**: logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)
- ... Additional arguments passed on to the `ExperimentHub-class` constructor

Details

The SCoPE2 study combines scRNA-seq (transcriptome) and single-cell proteomics.

- macrophage_differentiation: the cells are monocytes that undergo macrophage differentiation. No annotation is available for the transcriptome data, but batch and cell type annotations are available for the proteomics data in the `celltype` colData column. The transcriptomics and proteomics data were not measured from the same cells but from a distinct set of cell cultures. This dataset provides already filtered bad quality cells.
  - scRNAseq1 - single-cell transcriptome (batch 1)
  - scRNAseq2 - single-cell transcriptome (batch 2)
  - scp - single-cell proteomics

Value

A single cell multi-modal `MultiAssayExperiment` or informative data.frame when `dry.run` is TRUE

Source

All files are linked from the slavovlab website https://scope2.slavovlab.net/docs/data
References


See Also

SingleCellMultiModal-package

Examples

```r
SCoPE2(DataType = "macrophage_differentiation",
       modes = "*",
       version = "1.0.0",
       dry.run = TRUE)
```

Description

seqFISH function assembles data on-the-fly from ‘ExperimentHub’ to provide a MultiAssayExperiment container. Actually the ‘DataType’ argument provides access to the available datasets associated to the package.

Usage

```r
seqFISH(
    DataType = "mouse_visual_cortex",
    modes = "*",
    version,
    dry.run = TRUE,
    verbose = TRUE,
    ...
)
```

Arguments

- **DataType** character(1) indicating the identifier of the dataset to retrieve. (default "mouse_visual_cortex")
- **modes** character( ) The assay types or modes of data to obtain these include seq-FISH and scRNA-seq data by default.
- **version** character(1) Either version ’1.0.0’ or ’2.0.0’ depending on data version required (default ’1.0.0’). See version section.
- **dry.run** logical(1) Whether to return the dataset names before actual download (default TRUE)
verbose logical(1) Whether to show the dataset currently being (down)loaded (default TRUE)

... Additional arguments passed on to the ExperimentHub-class constructor

Details

seq FISH data are a combination of single cell spatial coordinates and transcriptomics for a few hundreds of genes. seq-FISH data can be combined for example with scRNA-seq data to unveil multiple aspects of cellular behaviour based on their spatial organization and transcription.

Available datasets are:

- mouse_visual_cortex: combination of seq-FISH data as obtained from Zhu et al. (2018) and scRNA-seq data as obtained from Tasic et al. (2016), Version 1.0.0 returns the full scRNA-seq data matrix, while version 2.0.0 returns the processed and subsetted scRNA-seq data matrix (produced for the Mathematical Frameworks for Integrative Analysis of Emerging Biological Data Types 2020 Workshop) The returned seqFISH data are always the processed ones for the same workshop. Additionally, cell types annotations are available in the ‘colData’ through the ‘class’ column in the seqFISH ‘assay’.
  - scRNA_Counts - Tasic scRNA-seq gene count matrix
  - scRNA_Labels - Tasic scRNA-seq cell labels
  - seqFISH_Coordinates - Zhu seq-FISH spatial coordinates
  - seqFISH_Counts - Zhu seq-FISH gene counts matrix
  - seqFISH_Labels - Zhu seq-FISH cell labels

Value

A MultiAssayExperiment of seq-FISH data

Author(s)

Dario Righelli <dario.righelli <at> gmail.com>

Examples

seqFISH(DataType = "mouse_visual_cortex", modes = "*", version = "2.0.0", dry.run = TRUE)

Description

Combine multiple single cell modalities into one using the input of the individual functions.
Usage

```r
SingleCellMultiModal(
  DataTypes,
  modes = "*",
  versions = "1.0.0",
  dry.run = TRUE,
  verbose = TRUE,
  ...
)
```

Arguments

- **DataTypes** character() A vector of data types as indicated in each individual function by the `DataType` parameter. These can be any of the following: "mouse_gastrulation", "pbmc_10x", "macrophage_differentiation", "cord_blood", "peripheral_blood", "mouse_visual_cortex", "mouse_embryo_8_cell"
- **modes** list() A list or CharacterList of modes for each data type where each element corresponds to one data type.
- **versions** character() A vector of versions for each `DataType`. By default, version `1.0.0` is obtained for all data types.
- **dry.run** logical(1) Whether to return the dataset names before actual download (default `TRUE`)
- **verbose** logical(1) Whether to show the dataset currently being (down)loaded (default `TRUE`)
- **...** Additional arguments passed on to the `ExperimentHub-class` constructor

Value

A multi-modality `MultiAssayExperiment`

metadata

The metadata in the `MultiAssayExperiment` contains the original function call used to generate the object (labeled as `call`), a `call_map` which provides traceability of technology functions to `DataType` prefixes, and lastly, R version information as `version`.

Examples

```r
SingleCellMultiModal(c("mouse_gastrulation", "pbmc_10x"),
  modes = list(c("acc*", "met*"), "rna"),
  version = c("2.0.0", "1.0.0"),
  dry.run = TRUE, verbose = TRUE
)
```
Index

* internal
  .CITEseqMaeToSce, 3
  .CITEseqMaeToSce, 3

addCTLabels, 4

CITEseq, 5

ExperimentHub-class, 5, 8, 12, 13, 15, 17, 18

getCellGroups, 7

GTseq, 8

MultiAssayExperiment, 5, 6, 8, 9, 12, 14–17

ontomap, 9

R_user_dir, 11

removeCache (scmmCache), 10

scmmCache, 10

scMultiome, 11

scNMT, 12

SCOPE2, 14

seqFISH, 16

setCache (scmmCache), 10

SingleCellMultiModal, 17

SingleCellMultiModal-package, 2